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Tellurene: a New Family of Two Dimensional Group-VI Monolayer Driven by Multivalency[1] YU JIA, ZHILI ZHU, XIAOLIN CAI, CHUNYAO NIU, School of Physics, Zhengzhou Univ., China, SEHO YI, JUN HYUNG CHO, Department of Physics, Hanyang Univ., Korea, ZHENGXIAO GUO, Department of Chemistry, UCL, UK, FENG LIU, Department of Mate. Sci. and Engin., Univ. of Utah, USA, ZHENGYU ZHANG, ICQD & HFNL, USTC, China — The exploration of two-dimensional (2D) layered materials is of fundamental and practical importance in contemporary condensed matter physics. Using the particle-swarm optimization method in combination with first-principles density functional theory calculations, we predict a new family of 2D monolayers composed of a group-VI element of Te. It is revealed that the multivalency character of Te plays a crucial role in forming monolayers with the 1T-MoS_2-like (termed α-Te), tetragonal (β-Te), and 2H-MoS_2-like (γ-Te) structures. We find that α- and β-Te are semiconductors, while γ-Te is metal. For α- and β-Te, the spin-orbit coupling effects give a transformation from an indirect band gap into a nearly direct and a direct band gap, respectively, leading to an optical absorption enhancement. Moreover, the semiconducting Te monolayers exhibit high electron and hole mobilities ranging from hundreds to thousands of $cm^2\,V^{-1}\,s^{-1}$, superior to MoS_2 monolayer. Our findings further extend the realm of 2D materials to include group-VI monolayers whose electronic properties are promising for potential applications in optoelectronics and electronics.

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